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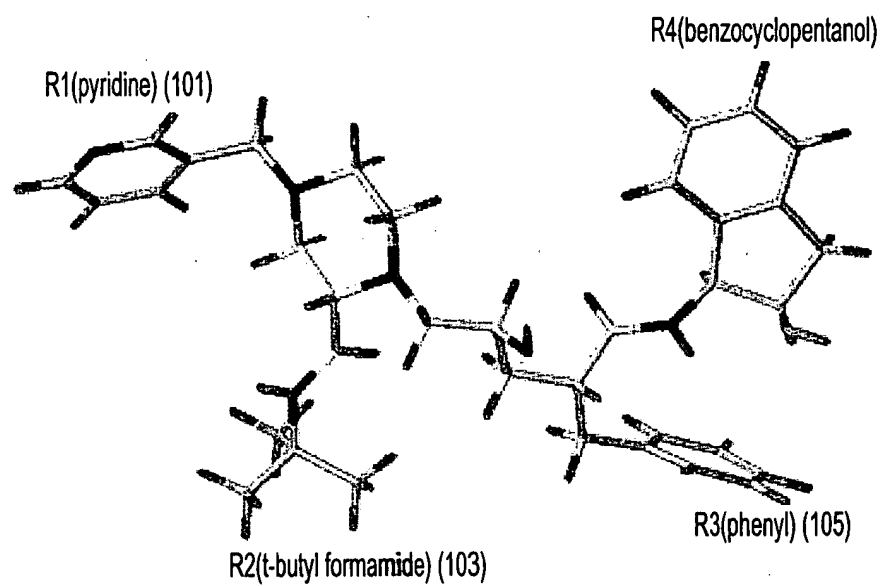
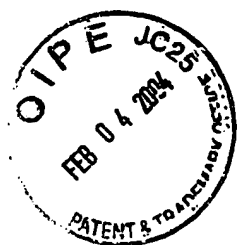


FIG. 1

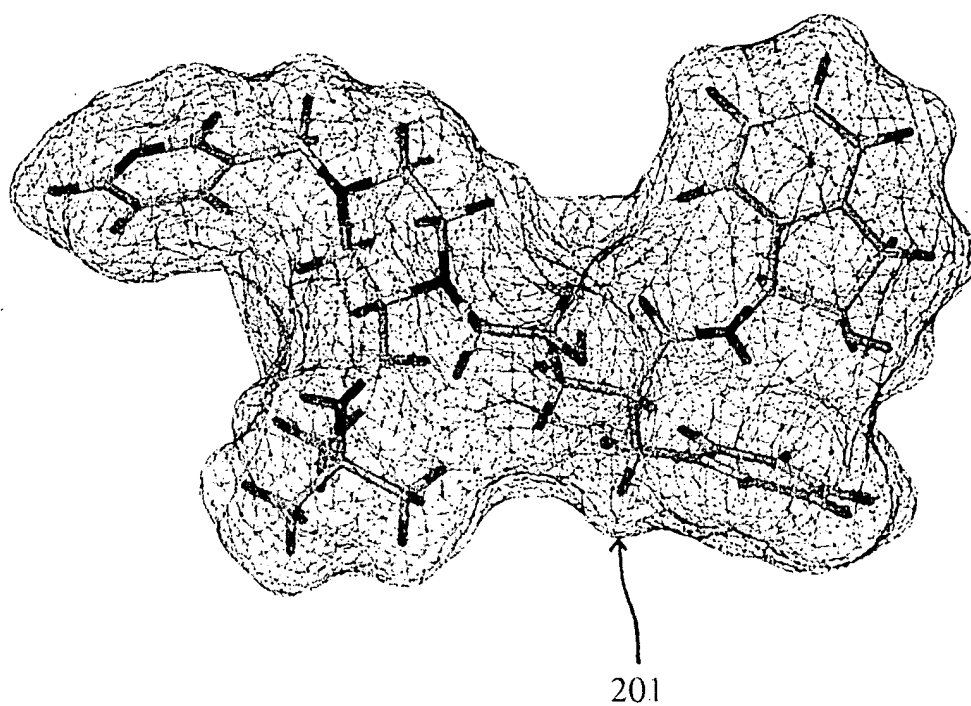


FIG. 2

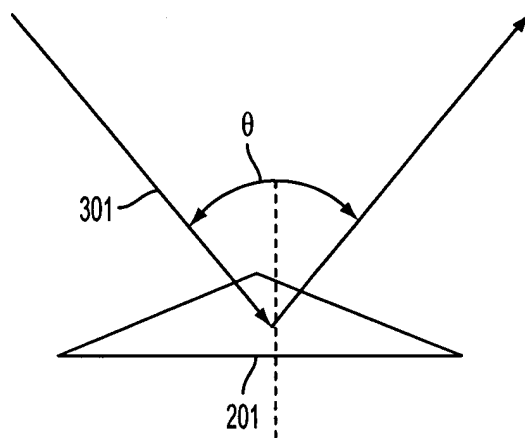


FIG. 3

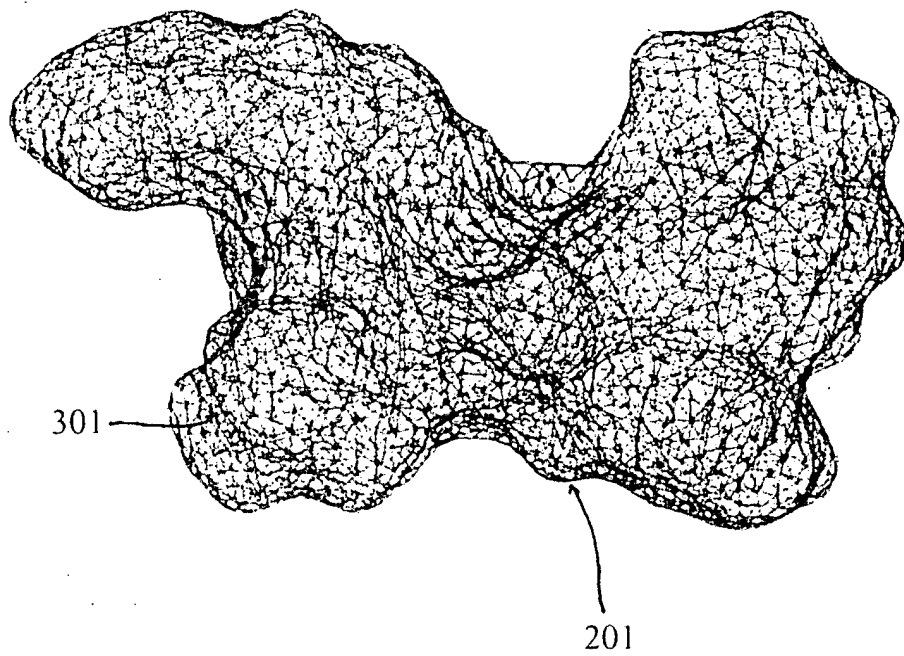


FIG. 4A

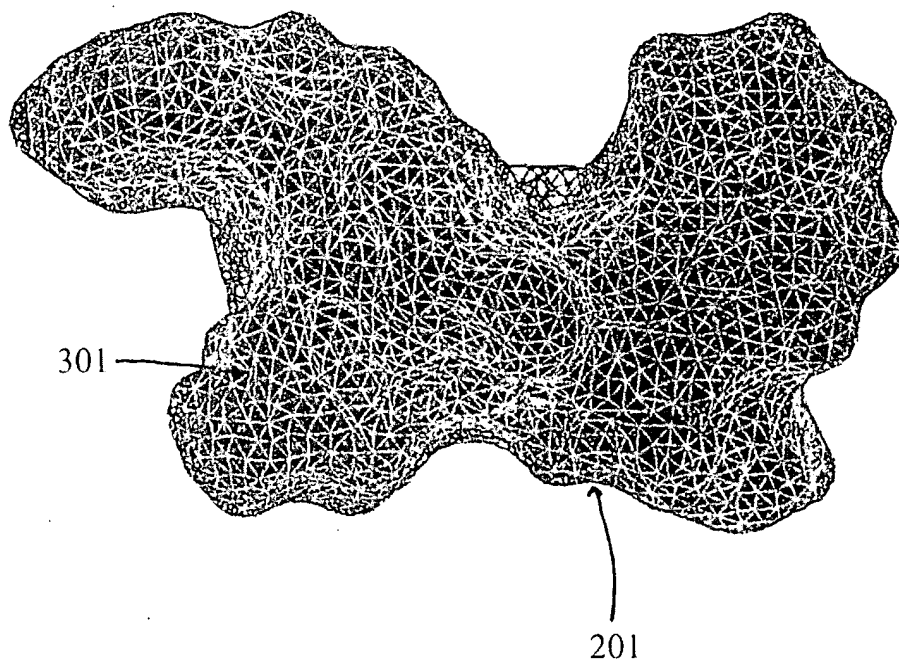


FIG. 4B

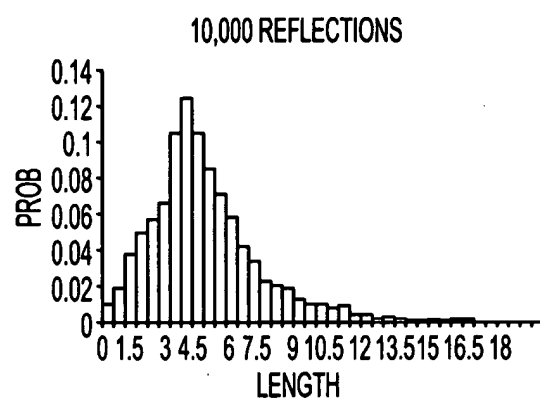


FIG. 5A

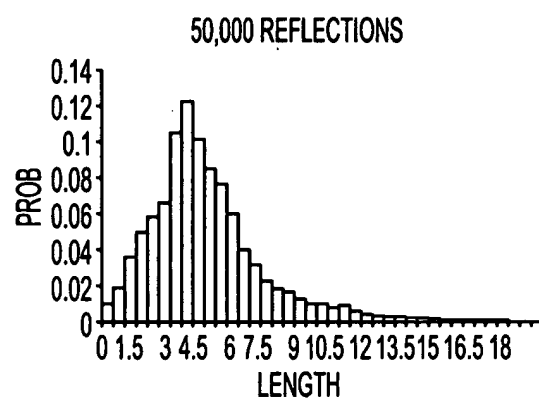


FIG. 5B

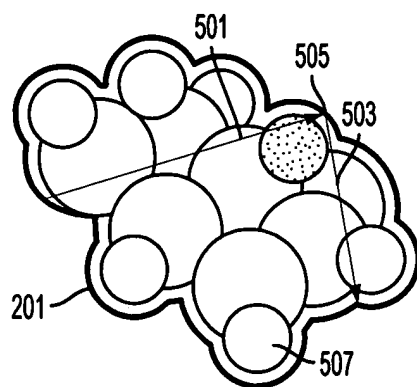


FIG. 6

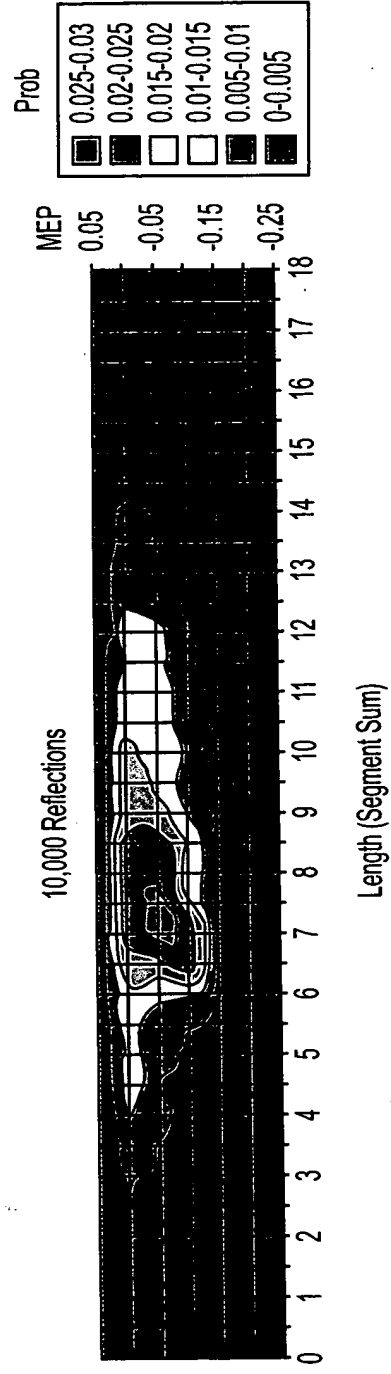


FIG. 7A

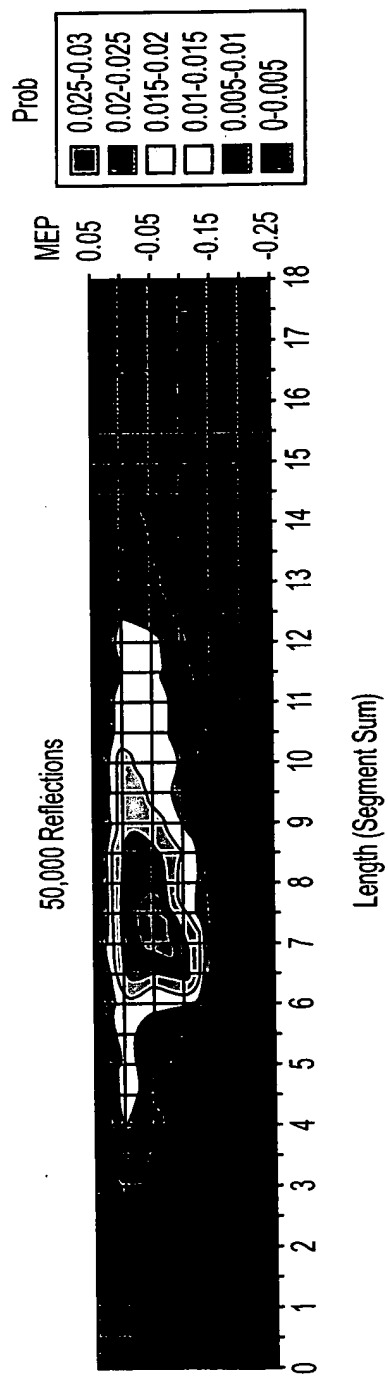


FIG. 7B

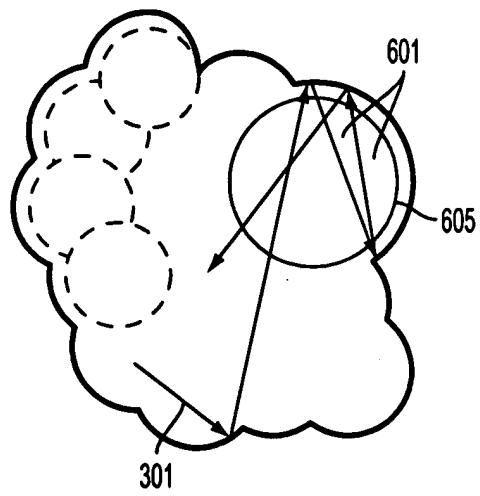


FIG. 8

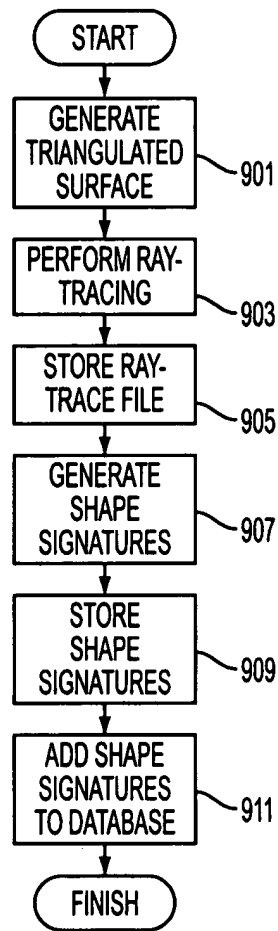


FIG. 9

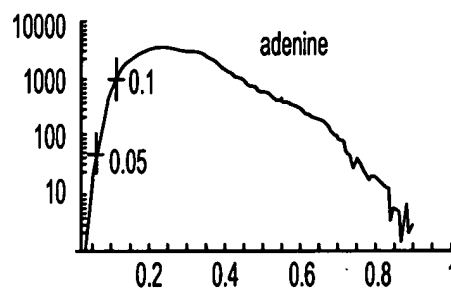
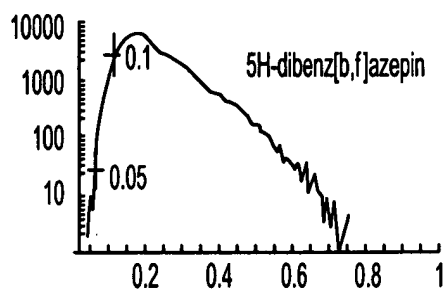
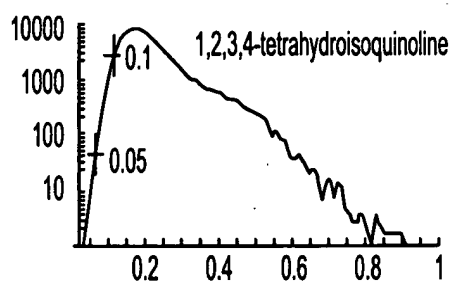


FIG. 10A

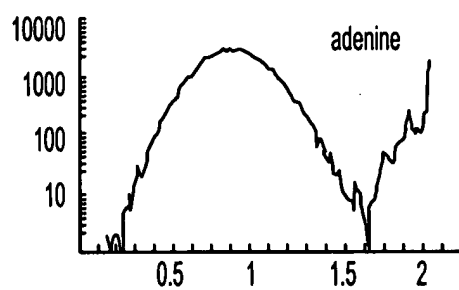
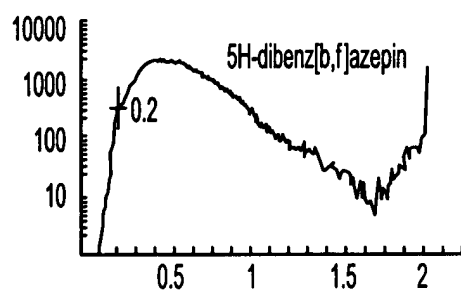
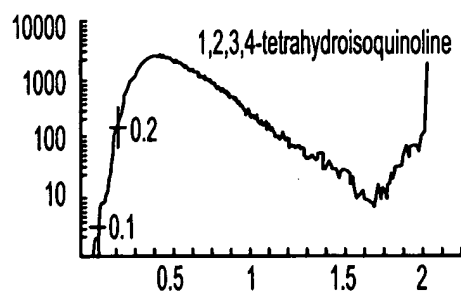


FIG. 10B

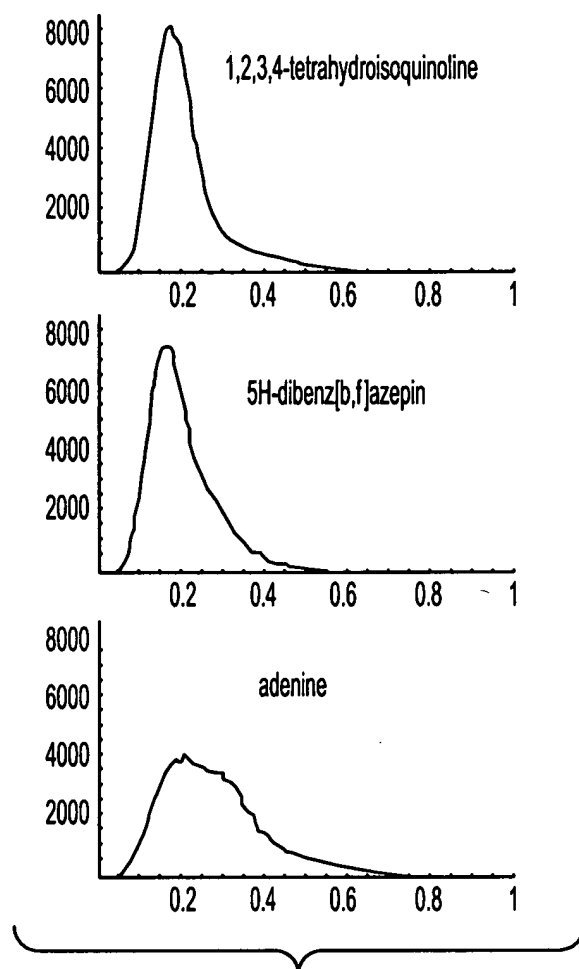


FIG. 11A

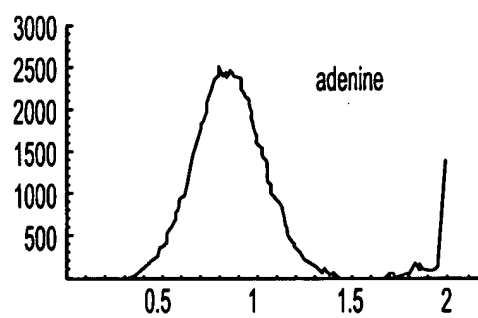
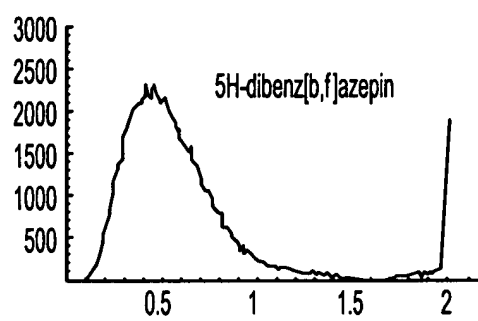
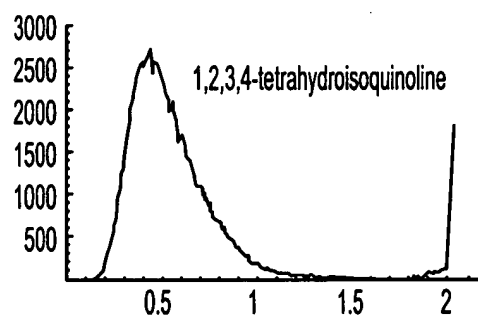


FIG. 11B

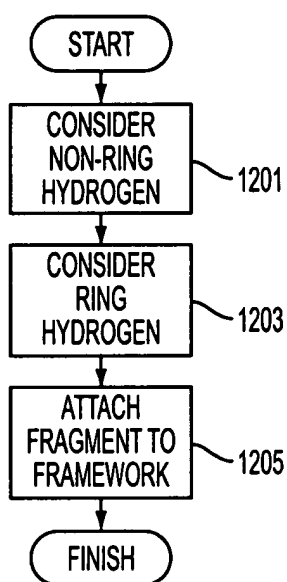


FIG. 12

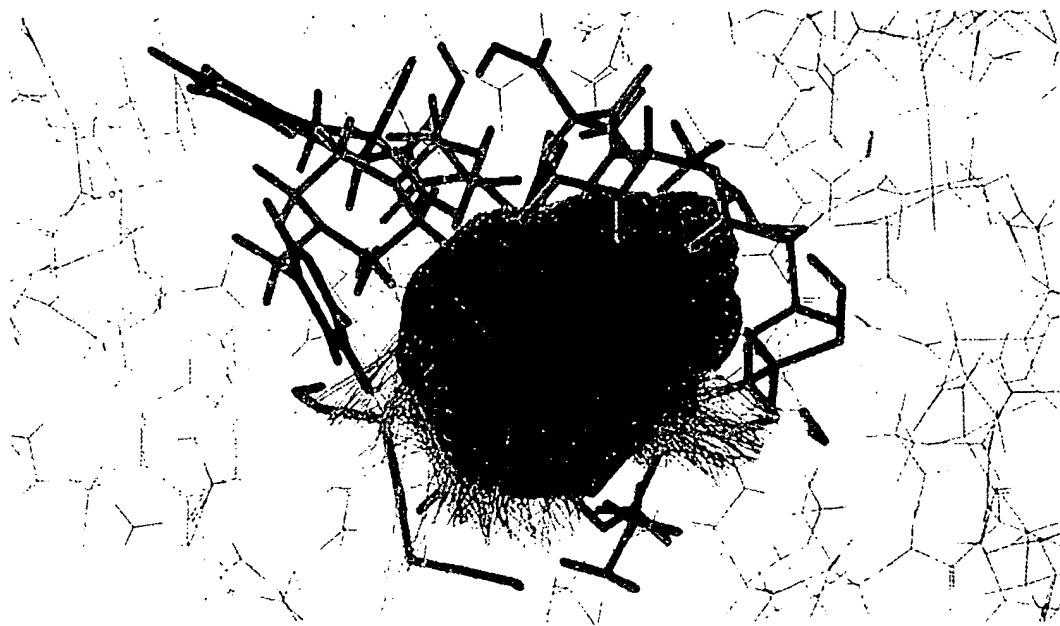


FIG. 13A

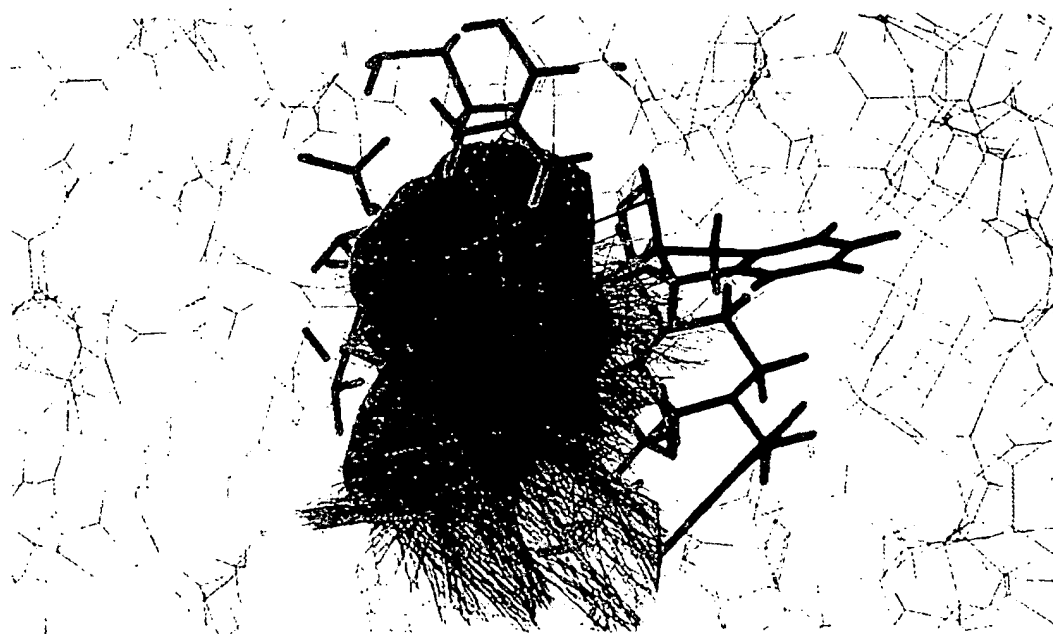


FIG. 13B

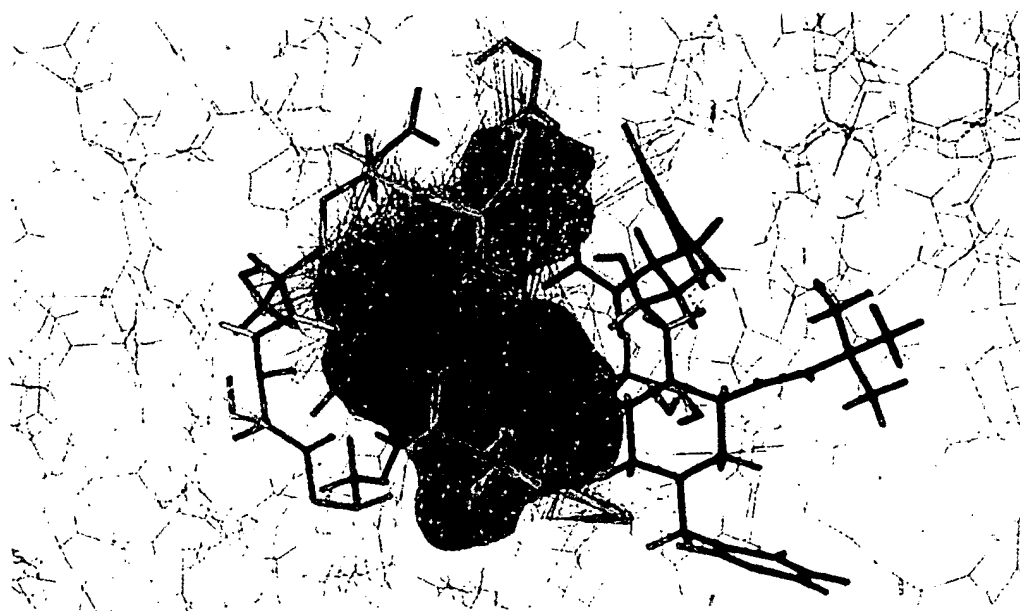


FIG. 13C

1,2,3,4-tetrahydroisoquinoline	1,2,3,4-tetrahydroquinoline isochroman 1,2,3,4-tetrahydronaphthalene chroman indoline	0.0370 0.0386 0.0490 0.0574 0.0767	1,2,3,4-tetrahydroquinoline isochroman chroman 1,2,3,4-tetrahydronaphthalene indan	0.0173 0.0316 0.0399 0.0475 0.0525
5H-dibenz[b,f]azepin	dibenzocycloheptatriene dihydrophenanthrene thioxanthene dibenz[b,f]thiepin 5H-dibenzo[b,f]-1,4-diazepine	0.0351 0.0482 0.0578 0.0695 0.0800	dibenzocycloheptatriene dihydrophenanthrene thioxanthene 5H-dibenzo[b,f]-1,4-diazepine dibenz[b,f]thiepin	0.0332 0.0384 0.0466 0.0487 0.0578
1,4,6-gonatriene-3,17-dione	4,6-gonadiene-3,17-dione 1,4-gonadien-3-one 4-gonen-3-one 1,3,5(10)-gonatriene 5(10)-gonen-3-one	0.0502 0.0743 0.0984 0.0986 0.1004	4,6-gonadiene-3,17-dione 1,4-gonadien-3-one 4-gonen-3-one 1,3,5(10)-gonatriene 5(10)-gonen-3-one	0.0400 0.0660 0.0838 0.0862 0.0984
α -D-glucopyranose	β -D-mannopyranose β -D-galactopyranose α -D-mannopyranose α -D-galactopyranose β -D-glucopyranose	0.0417 0.0420 0.0559 0.0744 0.0748	α -D-mannopyranose β -D-mannopyranose β -D-galactopyranose α -D-galactopyranose β -D-glucopyranose	0.0376 0.0379 0.0391 0.0560 0.0766
Lysine	Arginine Methionine Palmitoleate(C16) glycerol(-H) Olate(C18)	0.0862 0.1024 0.1163 0.1179 0.1202	Methionine Arginine Laurate(C12) Palmitoleate(C16) Myristate(C14)	0.0527 0.0821 0.0959 0.1004 0.1006
adenine	guanine 7H-purine cytosine uracil benzopyrimidine	0.0626 0.0712 0.0840 0.0854 0.0860	guanine 7H-purine benzimidazole 1H-indazole benzoxazole	0.0388 0.0701 0.0743 0.0747 0.0775

FIG. 14A









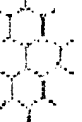


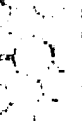
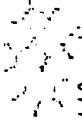



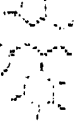
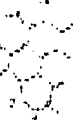



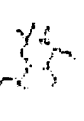
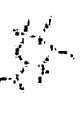




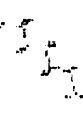

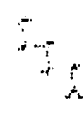



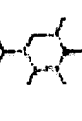
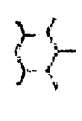

QUERIES	HIT #1	#2	#3	#4	#5
 1,2,3,4-tetrahydroisoquinoline	 1,2,3,4-tetrahydroquinoline	 isochroman	 1,2,3,4-tetrahydronaphthalene	 chroman	 indoline
 5H-dibenz[b,f]azepin	 dibenzocycloheptatriene	 dihydrophenanthrene	 thioxanthene	 dibenz[b,f]thiepin	 5H-dibenz[b,f]-1,4-diazepine
 1,4,6-gonatriene-3,17-dione	 4,6-gonadiene-3,17-dione	 1,4-gonadiene-3-one	 4-gon-3-one	 1,3,5(10)-gonatriene	 5(10)-gon-3-one
 α -D-glucopyranose	 β -D-mannopyranose	 β -D-glucopyranose	 α -D-mannopyranose	 α -D-galactopyranose	 β -D-glucopyranose
 Lysine	 Arginine	 Methionine	 Palmitoleate	 glycerol	 Oleate
 adenine	 guanine	 7H-purine	 cytosine	 uracil	 benzopyrimidine

FIG. 14B

L₁ Metric

QUERY	Culling		No Culling	
	Hit	Score	Hit	Score
1,2,3,4-tetrahydroisoquinoline	1,2,3,4-tetrahydroquinoline	0.0847	1,2,3,4-tetrahydroquinoline	0.0762
	1,2,3,4-tetrahydronaphthalene	0.1496	1,2,3,4-tetrahydronaphthalene	0.1307
	indoline	0.1732	indoline	0.1320
	acenaphthene	0.1908	indan	0.1554
	indan	0.2161	ace naphthene	0.1804
5H-dibenz[b,f]azepin	dibenzocycloheptatriene	0.1116	dibenzocycloheptatriene	0.1031
	acridan	0.2089	acridan	0.1538
	5H-dibenzo[b,f]-1,4-diazepine	0.2109	5H-dibenzo[b,f]-1,4-diazepine	0.1672
	1,2,3,4-tetrahydroisoquinoline	0.2268	phenanthridine	0.1762
	1,2,3,4-tetrahydroquinoline	0.2292	dihydrophenanthrene	0.1802
1,4,6-gonatriene-3,17-doine	4,6-gonadiene-3,17-dione	0.0888	4,6-gonadiene-3,17-dione	0.0852
	5a-gonane-3,17-dione	0.1383	5a-gonane-3,17-dione	0.1383
	1,4-gonadien-3-one	0.2028	1,4-gonadien-3-one	0.2097
	5a-gonan-3-one	0.2031	4-gonen-3-one	0.2122
	5a-gonan-17-one	0.2211	5a-gonan-3-one	0.2221
2-deoxy-β-D-ribofuranose	β-D-ribofuranose	0.2292	β-D-glucopyranose	0.2223
	β-D-glucopyranose	0.2368	α-D-fructofuranose	0.2317
	α-D-fructofuranose	0.2480	α-D-mannopyranose	0.2437
	α-D-galactopyranose	0.2616	β-D-ribofuranose	0.2445
	α-D-mannopyranose	0.2696	α-D-glucopyranose	0.2575
Lysine	Arginine	0.6615	Arginine	0.6617
	ethanolamine	0.7882	ethanolamine	0.7621
	choline	1.2682	choline	1.2442
	D-Thrcose	1.5332	D-Thrcose	1.4601
	D-Xylose	1.5667	D-Xylose	1.4912
adenine	pteridine	0.4025	benzothiazole	0.3493
	benzothiazole	0.4321	pteridine	0.3816
	guanine	0.4394	thiazole	0.3981
	7H-purine	0.4427	7H-purine	0.4254
	indene	0.4614	guanine	0.4265

FIG. 15

QUERY	L_1 Metric		R_1 Metric	
	Hit	Score	Hit	Score
1,2,3,4-tetrahydroisoquinoline	91-21-4	0.0291	91-21-4	0.1153
	10500-57-9	0.0336	10500-57-9	0.1409
	529-35-1	0.0348	578-54-1	0.1428
	578-54-1	0.0380	493-05-0	0.1534
	24206-39-1	0.0397	529-35-1	0.1743
5H-dibenz[b,f]azepin	833-48-7	0.0324	833-48-7	0.1404
	1211-06-9	0.0360	1211-06-9	0.1673
	10354-00-4	0.0415	10354-00-4	0.1789
	82-53-1	0.0441	42263-75-2	0.2142
	6279-16-9	0.0488	51087-02-6	0.2300
1,4,6-gonatriene-3,17-dione	24640-00-4	0.0450	6126-58-5	0.2289
	10448-96-1	0.0556	24640-00-4	0.2561
	438-67-5	0.0570	6968-06-5	0.2672
	5976-74-9	0.0576	20919-82-8	0.2908
	6126-58-5	0.0584	3601-97-6	0.2963
α -D-glucopyranose	488-66-4	0.0546	74561-03-8	0.2223
	23559-36-6	0.0548	488-66-4	0.2548
	74561-03-8	0.0553	488-64-2	0.2548
	16505-91-2	0.0607	6623-68-3	0.2548
	39392-65-9	0.0655	2037-48-1	0.2549
Lysine	5329-79-3	0.0478	37149-01-2	0.1874
	110-97-4	0.0486	6963-39-9	0.1882
	5343-35-1	0.0552	110-97-4	0.2107
	37149-01-2	0.0555	6281-43-2	0.2201
	7356-00-5	0.0563	104-50-7	0.2224
adenine	10325-61-8	0.0271	10325-61-8	0.0944
	54346-27-9	0.0304	54346-27-9	0.0988
	73-24-5	0.0310	5426-35-7	0.1178
	1123-54-2	0.0343	73-24-5	0.1178
	2227-98-7	0.0353	19165-47-0	0.1178

FIG. 16A


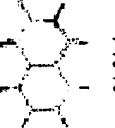
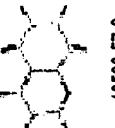

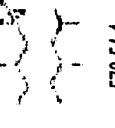
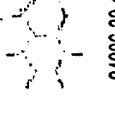

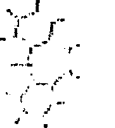



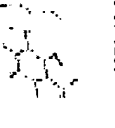

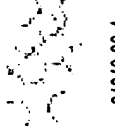
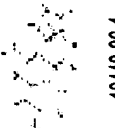
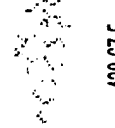
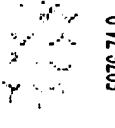
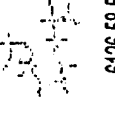

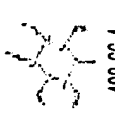
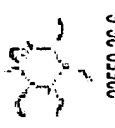
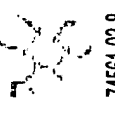
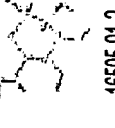
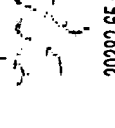
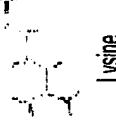
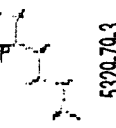
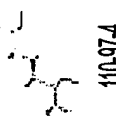
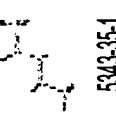
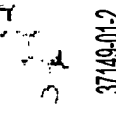
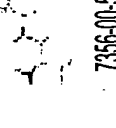


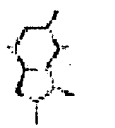



QUERIES	HIT #1	#2	#3	#4	#5
 1,2,3,4-tetrahydro- isoquinoline	 91-21-4	 10500-57-9	 529-35-1	 578-54-1	 24206-39-1
 5H-dibenz[b,f]- azepin	 833-48-7	 1211-06-9	 10354-00-4	 82-53-1	 6279-16-9
 1,4,6-gonatriene- 3,17-dione	 24640-00-4	 10448-96-1	 438-67-5	 5976-74-9	 6126-58-5
 α -D-glucopyranose	 488-66-4	 23559-36-6	 74561-03-8	 16505-91-2	 39382-65-9
 Lysine	 5329-79-3	 110-97-4	 5343-35-1	 37149-01-2	 7356-00-5
 adenine	 10325-61-8	 54346-27-9	 73-24-5	 1123-54-2	 2227-98-7

FIG. 16B

QUERY	L_1 Metric		R_1 Metric	
	Hit	Score	Hit	Score
1,2,3,4-tetrahydroisoquinoline	91-21-4	0.0701	91-21-4	0.5232
	635-46-1	0.0816	635-46-1	0.6553
	1484-19-1	0.0940	1484-19-1	0.6977
	1780-19-4	0.0983	5344-99-0	0.7295
	5344-99-0	0.1011	1780-19-4	0.8070
5H-dibenz[b,f]azepin	30646-39-0	0.0947	30646-39-0	0.8078
	16886-10-5	0.1079	3377-71-7	0.9075
	32446-13-2	0.1089	16886-10-5	0.9104
	3377-71-7	0.1126	32446-13-2	0.9166
	833-48-7	0.1167	833-48-7	0.9411
1,4,6-gonatriene-3,17-dione	56763-86-1	0.1524	20056-05-7	1.3418
	734-32-7	0.1645	56763-86-1	1.3451
	93998-31-3	0.1682	74924-17-7	1.4169
	20056-05-7	0.1693	734-32-7	1.4949
	74924-17-7	0.1702	71837-43-9	1.5131
α -D-glucopyranose	52019-14-4	0.1815	52019-14-4	1.4065
	49871-87-6	0.1833	58691-27-3	1.4270
	58691-27-3	0.1912	49871-87-6	1.4514
	7404-25-3	0.2015	2280-44-6	1.5418
	14215-77-1	0.2018	14215-77-1	1.5520
Lysine	42021-74-9	0.5473	85385-47-3	4.1381
	58048-33-2	0.5549	58048-33-2	4.2359
	58048-35-4	0.5684	42021-74-9	4.2441
	37082-52-3	0.5719	78582-26-0	4.3301
	78582-26-0	0.5721	62194-88-1	4.3458
adenine	73-24-5	0.0683	73-24-5	0.5048
	28128-33-8	0.1537	28128-33-8	1.0824
	7390-62-7	0.1581	7390-62-7	1.2106
	2846-89-1	0.1744	2846-89-1	1.2491
	3647-48-1	0.1820	1904-98-9	1.2947

FIG. 17A

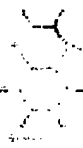

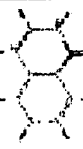



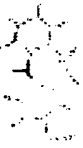
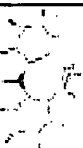








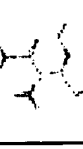

QUERIES	HIT #1	#2	#3	#4	#5
 1,2,3,4-tetrahydro- isoquinoline	 91-21-4	 635-46-1	 1484-19-1	 1780-19-4	 5344-99-0
 5H-dibenz[b,f]- azepin	 39646-39-0	 16886-10-5	 32446-13-2	 3377-71-7	 833-48-7
 adenine	 73-24-5	 28128-33-8	 7390-62-7	 2846-89-1	 3647-48-1

FIG. 17B

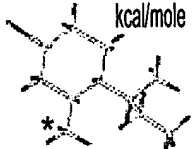

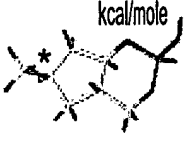

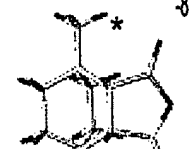
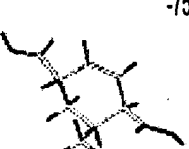
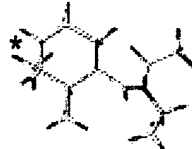

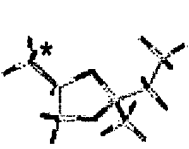


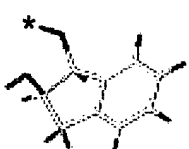
	R2	R3	R4
#1	 5396-90-7	 18650-61-8	 73581-87-0
#2	 62051-24-5	 26843-47-0	 19618-93-0
#3	 54243-68-4	 15298-66-5	 2916-28-1
Indinavir			

FIG. 18

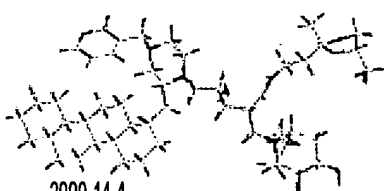
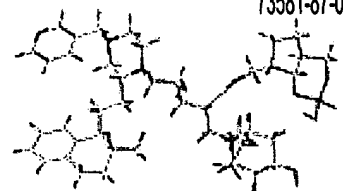
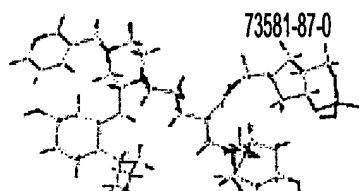
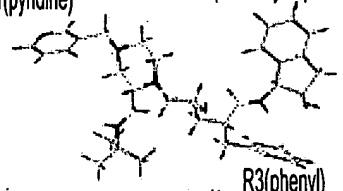
Rank	Energy(kcal/mol)	Structure
#1	-117.3	<div>2916-28-1</div>  <div>2090-14-4</div> <div>18650-61-8</div>
		<div>73581-87-0</div>  <div>5448-23-7</div> <div>18650-61-8</div>
		<div>73581-87-0</div>  <div>5396-90-7</div> <div>18650-61-8</div>
Indinavir	-97.2	<div>R1(pyridine)</div> <div>R4(benzocyclopentanol)</div>  <div>R2(t-butyl formamide)</div> <div>R3(phenyl)</div>

FIG. 19